

The importance of self-consistency in determining interface properties of $S - I - N$ and $D - I - N$ structures.

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(February 1, 2008)

Abstract

We develop a method to solve the Bogoliubov de Gennes equation for superconductors self-consistently, using the recursion method. The method allows the pairing interaction to be either local or non-local corresponding to s and d -wave superconductivity, respectively. Using this method we examine the properties of various $S - I - N$ and $D - I - N$ interfaces. In particular we self-consistently calculate the spatially varying density of states and the superconducting order parameter. We see that changing the strength of the insulating barrier, at the interface, does not, in the case of an s -wave superconductor, dramatically, change the low energy local density of states, in the superconducting region near the interface. This is in stark contrast to what we see in the case of a $D - I - N$ interface where the local particle density of states is changed dramatically. Hence we deduce that in calculating such properties as the conductance of $S - I - N$ and $D - I - N$ structures it is far more important to carry out a self-consistent calculations in the d -wave case.

I. INTRODUCTION.

The Bogoliubov de Gennes equations and approximations to these equations, for example the Eilenberger equations have in the last 10 years been used to great success to examine the properties of normal superconducting hybrid structures. Most of this work, in recent times, has centered upon solving these equations for the electrical mesoscopic transport properties of such hybrid structures for a recent review of calculations of electrical conductance properties of normal superconducting hybrid structures see Lambert and Ramondi [1]. Virtually all of this work has been centred around the properties of systems which contain conventional superconducting regions, ie. the superconducting gap has been isotropic. Also all but a few [2–12] have been non-self-consistent calculations, this however has not inhibited the success of such calculations. In more recent times, with the discovery of high-temperature superconductivity again the Bogoliubov de Gennes equations have been used to examine the properties of hybrid structures, where now the superconducting gap is taken to be non-isotropic, usually d -wave in symmetry, but mainly so far most of the theoretical analysis of *simple* experiments [13–15] have relied upon macroscopic symmetry arguments and not the microscopic details of the actual interfaces. However, the microscopic physics at the interface can be an important factor in understanding the experimental results. For example, if mixing of different order parameter symmetries occurs at the interface (because the interface breaks the bulk tetragonal or orthorhombic symmetry) the extent of such mixing can only be determined from microscopic calculations. Similarly, suppression of the order parameter (either d -wave or s -wave) near an $S - N$ interface can lead to significant local density of states within the bulk energy gap, and this can complicate the analysis of single electron tunnelling spectra [16].

In the past few years there have been a number of microscopic calculations of surfaces and interfaces in superconducting systems with a d -wave order parameter. Most of the theoretical results have been obtained using tunnelling theory, or Andreev's approximation [17–26] in which the tunnelling barrier and the order parameter are not found self-consistently. For tunnel junctions these approximations may be adequate, but we show below that self-consistency has significant effects for interfaces with direct contact between the constituents. Self-consistent properties of interfaces have previously been computed using the Eilenberger equations [27–32], which are an approximation to the Bogoliubov de Gennes equation. These self-consistent solutions to the Eilenberger equations have shown some interesting effects. Also there have now in the last couple of years been a few self-consistent calculations of the Bogoliubov de Gennes equations, with non-local interactions, looking at the effect of impurity scattering [33] and superconducting interfaces [34,35].

In this paper we tackle a *simple* problem, solving the Bogoliubov de Gennes equations self-consistently, in the presence of an s -wave and a d -wave order parameter with the aim of asking, how important is self-consistency? We present a method of how to calculate self-consistent properties of superconducting interfaces by directly solving the Bogoliubov de Gennes equations [35] and that certainly in the case of a d -wave interface it is crucial to perform such a calculation to obtain the correct form for the low energy density of states in the region of an interface. The method of performing our self-consistent calculations will be described in section II. Here we introduce the Bogoliubov de Gennes equation with a general interaction, U_{ij} , and demonstrate how this general Hamiltonian can be solved

self-consistently using the Recursion Method [36,37,35]. We then present results for bulk s -wave and d -wave systems; looking at both the local particle density of states and in the case of d -wave we look at the critical temperature as a function of band filling, we see that a d -wave solution, for the interaction we have chosen, is not the only possible solution, for our Hamiltonian.

Then in section III we present results for both $S - I - N$ and $D - I - N$ systems. We examine both the form of the superconducting order parameter in the region of the interface, for different strengths of insulating barrier, and how the local particle density of states varies in the region of the interface. What we see is the sub-gap local particle density of states, on the superconducting side of the interface, is not in the case of s -wave superconductivity effected by changing the strength of the insulating barrier, this is in marked contrast to what we see in the d -wave case. Finally in the conclusions we comment on what can be said in the light of our calculations.

II. THE BOGOLIUBOV DE GENNES EQUATION.

Our starting point is the non-local Hubbard model, which is described by the following Hamiltonian

$$H = - \sum_{ij\sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} - \mu \sum_{i\sigma} c_{i\sigma}^\dagger c_{i\sigma} + \frac{1}{2} \sum_{ij\sigma} U_{ij} c_{i\sigma}^\dagger c_{i\sigma} c_{j-\sigma}^\dagger c_{j-\sigma} \quad (1)$$

where the creation and annihilation operators $c_{i\sigma}^\dagger$ and $c_{i\sigma}$, respectively, create and annihilate electrons with spin σ in the orbital centred at the lattice point labelled by i , t_{ij} is the amplitude for hopping from site j to site i , μ is the chemical potential and U_{ij} is the interaction energy of two electrons with opposite spin on sites i and j . To obtain the, generalized non-local, Bogoliubov de Gennes Equation from equation (1) we first make a mean field approximation for the *pairing field*

$$\Delta_{ij} = -U_{ij} \langle c_{i\sigma} c_{j-\sigma} \rangle \quad (2)$$

and assuming that the fluctuations about this mean are small we then perform the Bogoliubov cononical-transformation, enabling us to obtain

$$\sum_j \mathbf{H}_{ij} \begin{pmatrix} u_j^n \\ v_j^n \end{pmatrix} = E_n \begin{pmatrix} u_i^n \\ v_i^n \end{pmatrix} \quad (3)$$

with

$$\mathbf{H}_{ij} = \begin{pmatrix} H_{ij} & \Delta_{ij} \\ \Delta_{ij}^* & -H_{ij}^* \end{pmatrix} \quad (4)$$

where u_i^n and v_i^n are the particle and hole amplitudes, on site i , associated with an eigenenergy E_n and where Δ_{ij} is the, possibly non-local, pairing potential or gap function, which does not have to be real.

In the fully self-consistent Bogoliubov de Gennes equation the normal state Hamiltonian H_{ij} is given by

$$H_{ij} = (t_{ij} + \frac{1}{2}U_{ij}n_{ij}) + (\epsilon_i - \mu)\delta_{ij} + \frac{1}{2}U_{ij}n_{jj} \quad (5)$$

where μ is the chemical potential, ϵ_i is the normal on site energy of site i and t_{ij} , as mentioned above is the hopping integral between site i and site j . The interaction terms $\frac{1}{2}U_{ij}n_{jj}$ and $\frac{1}{2}U_{ij}n_{ij}$ are the Hartree-Fock potentials, which are defined by

$$n_{ij} = \sum_{\sigma} \langle c_{i\sigma}^{\dagger} c_{j\sigma} \rangle = 2 \sum_n ((u_i^n)^* u_j^n f(E_n) + v_i^n (v_j^n)^* (1 - f(E_n))). \quad (6)$$

Similarly the pairing potentials are defined as

$$\Delta_{ij} = -U_{ij}F_{ij} \quad (7)$$

where the anomalous density is

$$F_{ij} = \langle c_{i\sigma} c_{j-\sigma} \rangle = \sum_n (u_i^n (v_j^n)^* (1 - f(E_n)) - (v_i^n)^* (u_j^n) f(E_n)). \quad (8)$$

In equations (6) the sum only considers terms E_n up to the condensate chemical potential (μ) as compared to equation (8) where the sum is over all terms.

A solution to the above system of equations will be fully self-consistent provided that both the normal ($U_{ij}n_{ij}$) and anomalous (Δ_{ij}) potentials are determined consistently with the corresponding densities n_{ij} and F_{ij} via equations (6) and (8).

Figure 1 illustrates the geometry corresponding to this system of equations, on a tight binding lattice. The tight-binding lattice has nearest neighbour hopping interactions (t_{ij}), as well as a coupling between particle and hole space, via a superconducting order parameter (Δ_{ij}). If the interactions are purely on-site (U_{ii}) attractions then the pairing potential will be purely local (Δ_{ii}), corresponding to the dashed line in figure 1. On the other hand when the interaction is non-local (U_{ij} , $i \neq j$) the pairing potential Δ_{ij} will also be non-local, as illustrated, for nearest neighbour interactions, by the solid lines in figure 1.

A. The Recursion Method for solving the Bogoliubov de Gennes Equations.

If we now wish to solve the Bogoliubov de Gennes equations self-consistently, we have found that the most efficient method of doing this is the Recursion Method [36]. This method allows us to calculate the electronic Green's functions

$$G_{\alpha\alpha'}(i, j, E) = \langle i\alpha | \frac{1}{E\mathbf{1} - \mathbf{H}} | j\alpha' \rangle \quad (9)$$

where the indices i and j denote sites, while α and α' represent the particle or hole degree of freedom on each site. We denote particle degrees of freedom by $\alpha = +$ and hole degrees of freedom by $\alpha = -$. For example $G_{+-}(i, j, E)$ represents the Greens function between the particle degree of freedom on site i and the hole degree of freedom on site j .

To compute the Green's functions (9) we can closely follow the method described by Litak, Miller and Györfy [37], they solved the Bogoliubov de Gennes Equation self-consistently, using the recursion method, for a local interaction. Using this method we can transform the Hamiltonian to a block tridiagonal form

$$E\mathbf{1} - \mathbf{H} = \begin{pmatrix} E\mathbf{1} - \mathbf{a}_0 & -\mathbf{b}_1 & 0 & 0 & 0 & 0 & 0 & \cdots \\ -\mathbf{b}_1^\dagger & E\mathbf{1} - \mathbf{a}_1 & -\mathbf{b}_2 & 0 & 0 & 0 & 0 & \cdots \\ 0 & -\mathbf{b}_2^\dagger & \ddots & \ddots & 0 & 0 & 0 & \cdots \\ 0 & 0 & \ddots & \ddots & \ddots & 0 & 0 & \cdots \\ 0 & 0 & 0 & -\mathbf{b}_n^\dagger & E\mathbf{1} - \mathbf{a}_n & -\mathbf{b}_{n+1} & 0 & \cdots \\ \vdots & \vdots & \vdots & 0 & \ddots & \ddots & \ddots & \ddots \end{pmatrix} \quad (10)$$

where \mathbf{a}_n and \mathbf{b}_n are 2×2 matrices. Given this form for $\langle i\alpha | E\mathbf{1} - \mathbf{H} | j\alpha' \rangle$ and expressing the Green's function as

$$G_{\alpha\alpha'}(i, j, E) = \langle i\alpha | (E\mathbf{1} - \mathbf{H})^{-1} | j\alpha' \rangle, \quad (11)$$

the Greens functions above can be evaluated as a matrix continued fraction so that

$$\mathbf{G}(i, j, E) = \left(E\mathbf{1} - \mathbf{a}_0 - \mathbf{b}_1^\dagger \left(E\mathbf{1} - \mathbf{a}_1 - \mathbf{b}_2^\dagger \left(E\mathbf{1} - \mathbf{a}_2 - \mathbf{b}_3^\dagger (E\mathbf{1} - \mathbf{a}_3 - \dots)^{-1} \mathbf{b}_3 \right)^{-1} \mathbf{b}_2 \right)^{-1} \mathbf{b}_1 \right)^{-1} \quad (12)$$

where

$$\mathbf{G}(i, j, E) = \begin{pmatrix} G_{\alpha\alpha}(i, i, E) & G_{\alpha\alpha'}(i, j, E) \\ G_{\alpha'\alpha}(j, i, E) & G_{\alpha'\alpha'}(j, j, E) \end{pmatrix}. \quad (13)$$

Within equations (10) and (12) we have a formally exact representation of the Green's functions. However in general both the tridiagonal representation of the Hamiltonian, and the matrix continued fraction (10) will be infinite. In practice one can only calculate a finite number of terms in the continued fraction exactly. In the terminology of the recursion method it is necessary to *terminate* the continued fraction [36–42].

If we were to calculate up to and including \mathbf{a}_n and \mathbf{b}_n and then simply set subsequent coefficients to zero then the Green's function would have $2n$ poles along the real axis. The density of states would then correspond to a set of $2n$ delta functions. Integrated quantities such as the the densities n_{ij} and F_{ij} could depend strongly on n , especially since only a few of the $2n$ delta functions would be within the relevant energy range within the BCS cut off, E_c . In order to obtain accurate results it would be necessary to calculate a large number of exact levels, which would be expensive in terms of both computer time and memory.

As a more efficient alternative we choose to terminate the continued fraction using the extrapolation method, as used previously by Litak, Miller and Györffy [37]. We calculate the values for \mathbf{a}_n and \mathbf{b}_n exactly up to the first m coefficients using the recursion method. Then, noting the fact that the elements of the matrices \mathbf{a}_n and \mathbf{b}_n vary in a predictable manner [37], we extrapolate the elements of the matrices for a further k iterations, where k is usually very much greater than m . This enables us to compute the various densities of states, and the charge densities n_{ij} and F_{ij} accurately with relatively little computer time and memory.

In terms of the Green's functions $G_{\alpha\alpha'}(i, j, E)$ the pairing and normal Hartree-Fock potentials Δ_{ij} and $\frac{1}{2}U_{ij}n_{ij}$ can be expressed as

$$\Delta_{ij} = \frac{1}{2\pi} U_{ij} \int (G_{+-}(i, j, E + \eta) - G_{+-}(i, j, E - \eta))(1 - 2f(E)) dE \quad (14)$$

and

$$\frac{1}{2} U_{ij} n_{ij} = \frac{1}{2\pi} U_{ij} \int (G_{++}(i, j, E + \eta) - G_{++}(i, j, E - \eta)) f(E) dE \quad (15)$$

where η is a small positive number.

To obtain the above equations we have used the fact that

$$\begin{pmatrix} u_i^n \\ v_i^n \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} -(v_i^n)^* \\ (u_i^n)^* \end{pmatrix} \quad (16)$$

are the eigenvectors of equation (3) with eigenvalues E_n and $-E_n$.

It should be noted that up to this point we have been completely general, so we are not just restricted to calculating the Greens functions on the same site, $G_{\alpha\alpha'}(i, i, E)$ or just between nearest neighbours, in essence we could use this formalism to calculate a Greens function between any two sites. This enables us to also calculate such quantities as $G_{++}(i, j, E)$ and $G_{+-}(i, j, E)$, which can then in turn be used to calculate normal reflection and transmission coefficients, thus enabling in principle for transport properties or our Hamiltonian to be calculated.

B. Achieving Self-consistency.

Using the above methods to calculate Δ_{ij} and $U_{ij}n_{ij}$ we need to achieve a fully self-consistent solution. Firstly we make use of any symmetries in the system in order to minimise the number of calculations which are necessary. For example on an infinite square lattice with no variation in any of the potentials only one independent site needs to be calculated since this site can be mapped onto all of the other sites. Secondly, once we have decided which sites need to be calculated self-consistently Δ_{ij} and n_{ij} can be calculated for those sites, remembering that on a square lattice each site will have four nearest neighbours. This implies that in general we will have to calculate nine different Green's functions in order to calculate Δ_{ij} and n_{ij} . This can be seen by considering site i in figure 1 and noting that we need to calculate the Greens functions shown in table I, depending on whether the interaction is purely local, purely non-local, or both local and non-local. Having calculated the appropriate Green's functions new values for Δ_{ij} and n_{ij} can be calculated, which we will denote as $\Delta_{ij}^{(1)}$ and $n_{ij}^{(1)}$. Inserting these into the Hamiltonian and repeating the calculation of then Green's functions leads to a new set $\Delta_{ij}^{(2)}$ and $n_{ij}^{(2)}$ and so on. We repeat this iteration for all i and j until

$$\left| \frac{|\Delta^{(n-1)}| - |\Delta^{(n)}|}{|\Delta^{(n)}|} \right| \leq 0.001 \quad (17)$$

and

$$\left| \frac{|n^{(n-1)}| - |n^{(n)}|}{|n^{(n)}|} \right| \leq 0.001. \quad (18)$$

Since Δ_{ij} and n_{ij} can be complex we need to also check for convergence in their associated phases.

C. Uniform properties of our Hamiltonian.

Up to this point we have said nothing about the interaction itself, just that it exists. In conventional BCS theory [43] we can impose a cut-off for our interaction, since we know that in this case the interaction is phonon mediated, thus in equations (14) and (16) we can have a cut-off for our integrals. However we also wish to consider the properties of high-temperature superconductors, where the mechanism for the interaction is a controversial area, so we state at this point that we are not interested in the mechanism for high-temperature superconductivity, but we do know, through experiment [44], that the symmetry of the superconducting order parameter in high-temperature materials is of a d -wave nature, therefore, generally we wish to consider the properties of d -wave superconductors.

The simplest model to consider is one where we have a nearest neighbour attractive interaction, U_{ij} . For such a situation, where the interaction is constant we can calculate the critical temperature for a given interaction strength, as a function of band filling, see figure 2. It is found that there are two possible solutions for the symmetry of the superconducting order parameter. In this figure we can see there are two critical temperatures, one for extended s -wave solutions, near the edges of the band, and a d -wave solution near the centre of the band. It is this d -wave solution which we will be considering, however it is important to note, and will be seen later, that in non-uniform systems although we may be at a band filling where only the d -wave solution exists this does not necessitate that the extended s -wave components to the superconducting order parameter will thence be zero.

Before proceeding it is instructive to examine the bulk local particle density of states ($N(E)$) for the systems we are concerned with. In figure 3 we have plotted the local particle density of states,

$$N_i(E) = \frac{1}{2\pi}(G_{++}(i, i, E + \eta) - G_{++}(i, i, E - \eta)). \quad (19)$$

for three different scenarios, no interaction (thin dashed line), a local interaction (thin solid line) and a, nearest neighbour, non-local interaction (thick solid line). What we see from this is exactly what one would expect, i.e. for no interaction, we obtain the density of states for a regular, nearest neighbour tight binding lattice, for a local interaction we obtain a BCS type gap centred around the Fermi Energy, and finally for a non-local interaction we see a typical d -wave gap, i.e. the local particle density of states goes to zero linearly at the Fermi energy. Having said that there is no way, at this point to discern that we actually have a d -wave solution, but we define a d -wave order parameter in the following manner

$$|\Delta_i^{(d)}| = \frac{1}{4}|\Delta_{ij_1} - \Delta_{ij_2} + \Delta_{ij_3} - \Delta_{ij_4}|, \quad (20)$$

where j_1, j_2, j_3 and j_4 are the nearest neighbours to i , moving in a clockwise or anticlockwise direction, this quantity is then the d -wave component to the order parameter at i , similarly we can also write

$$|\Delta_i^{(s)}| = \frac{1}{4}|\Delta_{ij_1} + \Delta_{ij_2} + \Delta_{ij_3} + \Delta_{ij_4}| \quad (21)$$

for the extended s -wave component to the order parameter. For the results obtained in figure 3 $|\Delta_i^{(d)}| = 0.38 * t$ and $|\Delta_i^{(s)}| = 0$.

III. RESULTS FOR $S - I - N$ AND $D - I - N$ INTERFACES

Now we can proceed to perform self-consistent calculations for interfaces. Our *model* is as follows, we consider a system which does not vary in the y coordinate and has a step like function in the interaction strength in the x coordinate; ie. for $x < 0$ the interaction is finite; whereas for $x \geq 0$ our interaction (be it local or nearest neighbour non-local) is zero. The interface itself is modelled by a line of sites at $x = 0$, where we change the on-site energy of these sites in accordance with the strength of the barrier at the interface we wish to model. We then proceed to calculate the Bogoliubov de Gennes equations in the self-consistent manner prescribed above.

First we look at the results obtained for a local interaction ($U_{ii} = -1.5t$). We see in figure 4 the nomalized magnitude of the superconducting order parameter (upper graph) and $\frac{1}{2}U(x)n(x)$ (lower graph), where in reference to the prevoius equations we have made a transformation from sites i to position x . In this figure we see how these two quantities vary in the region of the interface ($x = 0$), for different strengths of the barrier at the interface, $\epsilon(0) = 0$ (thin solid line), $\epsilon(0) = 0.5t$ (thin dashed line), $\epsilon(0) = 1.0t$ (thick solid line) and $\epsilon(0) = 2.0t$ (thick dashed line). The main point to deduce from this is that the barrier has very little effect upon the actual order parameter or the local density. This is in comparison to what we see for an equivalent calculation for a non-local interaction, the results of which are shown in figure 5, where we have plotted the nomalised d -wave contribution to the superconducting order parameter (upper graph) and the extended s -wave contribution to the superconducting order parameter (lower graph), for the same interface configurations as used to obtain figure 4. What we see here is that although $\Delta^{(d)}(x)$ is not seroiusly modified in the presence of a barrier, $\Delta^{(s)}(x)$ is. We can see that as we increase the strength of the barrier $\Delta^{(s)}(x)$ in the region of the interface is reduced.

We now wish to focus our attention on the local particle density of states, near the interface. How this quantity changes will be important in deducing whether it is crucial to perform self-consistent calculations to obtain quantities which are reliant upon the local particle density of states near the interface. As an example we are going to focus on the sub-gap density of states and how this changes for different barrier strengths, and whether it is then valid to use non-self-consistent calculations in calculating such quantities as the sub-gap conductance?

With this in mind we have in figure 6 plotted the low energy local particle density of states for a local interaction ($U_{ii} = -1.5t$), at $x = -2$. We have plotted this quantity for different strengths of barrier, $\epsilon(0) = 0$ (thin dashed line), $\epsilon(0) = 0.5t$ (thin solid line), $\epsilon(0) = 1.0t$ (thick dashed line), $\epsilon(0) = 2.0t$ (thick solid line) and $\epsilon(0) = 3.0t$ (thin dashed-dotted line). Again, as in figure 4 there is little change in the quantity we are interested in. In fact from this plot we can say that a quantity such as the sub-gap, $S - I - N$ conductance depends very little on changes in the density of states and is totally governed by the tunnelling conductance of the barrier.

However again taking the d -wave case we can see an altogther different story. In figure 7 we have plotted equivalent local particle density of states as in figure 6, but for a d -wave interface. What we see is that the low energy density of states in the region of the barrier is modified significantly, when we change the strength of the barrier, and hence we can no longer state that the conductance of an $D - I - N$ interface will be mainly governed

by the tunnelling conductance of the barrier. This implies that in such calculations, when comparing, for example the conductances of different $D - I - N$ interfaces, the details of the barrier effect the sub-gap density of states on the superconducting side of the barrier and hence self-consistency has an important role to play.

Finally to highlight the point that the low energy local particle density of states in the region of an interface is modified significantly, by the strength of the barrier at the interface, when the superconducting region has a d -wave symmetry, we have in figure 8 plotted the local particle density of states at $x = -1$ (a), $x = -2$ (b), $x = -3$ (c) and $x = -4$ (d). for two different strengths of barrier $\epsilon(0) = 0$ (thin solid line) and $\epsilon = 3.0t$ (thick solid line). From this figure we can see the *dramatic* change in the sub-gap local density of states. Particularly in figure 8(a) (nearest the interface) we see that in the region of $E = 0$, when there is no interface barrier, there is always a significant density of states at the interface, as compared to $N(0) \approx 0$ when we have a finite barrier.

IV. CONCLUDING REMARKS.

In this paper we have developed the Recursion Method for calculating the Bogoliubov de Gennes equations self-consistently with both local and non-local interactions. Then as a *simple* problem we examined the self-consistent local particle density of states in the region of both $S - I - N$ and $D - I - N$ interfaces, in particular we have focused on how the local particle density of states is modified as we change the strength of the barrier. What we see is that in the case of the $S - I - N$ interface the low energy particle density of states, on the superconducting side of the interface, does not change dramatically as we change the strength of the insulating barrier. This is in stark contrast to the comparatively dramatic change we see when we perform the same calculation for a $D - I - N$ interface.

These results imply that in the case of d -wave interfaces the details of the the interface are important and hence to get these details correct we should perform a self-consistent calculation. If we do a non-self-consistent calculation for the case of the d -wave interface, i.e. just let the order parameter vary in a step like manner at the interface, then we see that the low energy density of states on the superconducting side of the barrier is unaltered as we change the strength of the insulating barrier, at the interface. This discrepancy, between self-consistent and non-self-consistent calculations, arises from the fact that we have a mixing of symmetries in the region of the self-consistent d -wave interface and when a self-consistent calculation is performed we see that this mixing changes as the interface is changed, this effect will not be seen in a non-self-consistent calculation.

These results may well explain why non-self-consistent conductance calculations for hybrid s -wave structures have over the past years been so successful, i.e the problem can simply be seen as calculating the tunnel conductance of the barrier, but also raises a warning flag that such a bold approach for d -wave structures may not be as effective, since our calculations show that the low energy density of states changes as we change the properties of the interface, we believe that the only way to obtain the correct low energy density of states behaviour is to perform a self-consistent calculation.

V. ACKNOWLEDGMENTS.

This work was supported by the EPSRC under grant number GR/L22454 and by the TMR network Dynamics of Nanostructures. We would like to thank B.L Györfy for useful discussions.

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FIGURES

FIG. 1. This is a schematic diagram of a tight binding lattice, with particle and hole degrees of freedom, Δ_{ij} couples particles on site i to holes on site j . The difference between local and non-local pairing is highlighted by the dashed (local pairing) and solid (non-local pairing) lines.

FIG. 2. The critical temperature vs. band filling for a fixed non-local, nearest neighbour interaction, the dashed line is the extended s -wave solution to the linearized gap equation and the solid line is the corresponding d -wave solution.

FIG. 3. The local particle density of states for a 2-D tight binding lattice, with no interactions ($U_{ij} = 0$) (thin dashed line), with a local interaction ($U_{ii} = 1.5t$) (thin solid line) and finally with a non-local nearest neighbour interaction ($U_{ij} = 1.5t$) (thick solid line). For this system $t_{ij} = 1$ for nearest neighbours only, $\mu = 0$ and $\epsilon_i = 0$.

FIG. 4. The magnitude of the superconducting order parameter (upper graph), normalised to the magnitude at $x = -\infty$ and $1/2U(x)n(x)$ (lower graph), as a function of x , where we have an interface at $x = 0$. Each of the lines on the upper and lower graphs are for different strengths of barrier at $x = 0$, $\epsilon(0) = 0$ (thin solid line), $\epsilon(0) = 0.5t$ (thin dashed line), $\epsilon(0) = 1.0t$ (thick solid line) and $\epsilon(0) = 2.0t$ (thick dashed line).

FIG. 5. The magnitude of the d -wave component to the superconducting order parameter normalized to its value at $x = -\infty$ (upper graph) and the s -wave component to the superconducting order parameter (lower graph) as a function of x , for different strengths of barrier at $x = 0$. We have $\epsilon(0) = 0$ (thin solid line), $\epsilon(0) = 0.5t$ (thin dashed line), $\epsilon(0) = 1.0t$ (thick solid line) and $\epsilon(0) = 2.0t$ (thick dashed line).

FIG. 6. The local particle density of states, at $x = -2$, for an attractive local interaction, for $x < 0$. The different lines are again for different strengths of interaction, $\epsilon(0) = 0$ (thin dashed line), $\epsilon(0) = 0.5t$ (thin solid line), $\epsilon(0) = 1.0t$ (thick dashed line), $\epsilon(0) = 2.0t$ (thick solid line) and $\epsilon(0) = 3.0t$ (thin dashed-dotted line).

FIG. 7. The local particle density of states, at $x = -2$, for an attractive non-local interaction, for $x < 0$. The different lines are again for different strengths of interaction, $\epsilon(0) = 0$ (thin dashed line), $\epsilon(0) = 0.5t$ (thin solid line), $\epsilon(0) = 1.0t$ (thick dashed line), and $\epsilon(0) = 2.0t$ (thick solid line) (thin dashed-dotted line).

FIG. 8. The local particle density of states, at $x = -1$ (a), $x = -2$ (b), $x = -3$ (c) and $x = -4$ (d), for an attractive non-local interaction, for $x < 0$. The different lines are again for different strengths of interaction, $\epsilon(0) = 0$ (thin solid line), and $\epsilon(0) = 3.0t$ (thick solid line).

TABLES

Interaction Type	$\mathbf{G}_{+-}(i, i, E)$	$\mathbf{G}_{+\pm}(i, j_1, E)$	$\mathbf{G}_{+\pm}(i, j_2, E)$	$\mathbf{G}_{+\pm}(i, j_3, E)$	$\mathbf{G}_{+\pm}(i, j_4, E)$
U_{ii}	Y	N	N	N	N
$U_{ij}(1 - \delta_{ij})$	N	Y	Y	Y	Y
$U_{ii} + U_{ij}(1 - \delta_{ij})$	Y	Y	Y	Y	Y

TABLE I. This table shows which Greens functions need to be calculated for systems with interactions which are local, U_{ii} , non-local, $U_{ij}(1 - \delta - ij)$, or both. The site labels correspond to the notation of Fig. 1.















